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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1	JUN 06	Web Page for STN Seminar Schedule - N. America
NEWS 2	JUN 06	EFFULL enhanced with 260,000 English abstracts
NEWS 3	JUN 06	KOREPAT updated with 41,000 documents
NEWS 4	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS 5	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS 6	JUN 25	CA/Cplus and USPAT databases updated with IPC reclassification data
NEWS 7	JUN 30	AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS 8	JUN 30	EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS 9	JUN 30	STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS 10	JUN 30	STN AnaVist enhanced with database content from EPFULL
NEWS 11	JUL 28	CA/Cplus patent coverage enhanced
NEWS 12	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS 13	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS 14	JUL 28	STN Viewer performance improved
NEWS 15	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS 16	AUG 13	CA/Cplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS 17	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS 18	AUG 15	Cplus currency for Korean patents enhanced
NEWS 19	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS 20	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS 21	SEP 25	CA/Cplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS 22	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and Korean patents enhanced
NEWS 23	SEP 29	IFICLS enhanced with new super search field
NEWS 24	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS 25	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents

NEWS 26 OCT 07 EPFULL enhanced with full implementation of EPC2000  
NEWS 27 OCT 07 Multiple databases enhanced for more flexible patent  
number searching

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,  
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 10:00:42 ON 20 OCT 2008

=> file reg  
COST IN U.S. DOLLARS  
SINCE FILE ENTRY SESSION  
0.21 0.21  
FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:00:50 ON 20 OCT 2008  
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 OCT 2008 HIGHEST RN 1063403-85-9  
DICTIONARY FILE UPDATES: 19 OCT 2008 HIGHEST RN 1063403-85-9

New CAS Information Use Policies, enter HELP.USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008

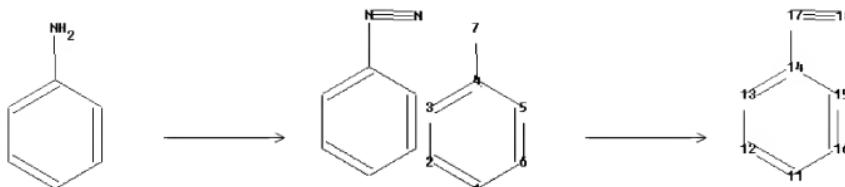
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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stn/gen/stndoc/properties.html>

22

Uploading C:\Program Files\STNEXP\Queries\10559834 uncharged.str



chain nodes :

7 17 18

ring nodes :

1 2 3 4 5 6 11 12 13 14 15 16

chain bonds :

4-7 14-17 17-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

exact/norm bonds :

4-7 14-17 17-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

isolated ring systems :

containing 1 : 11 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 11:Atom 12:Atom 13:Atom  
14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

fragments assigned reactant/reagent role:

containing 1

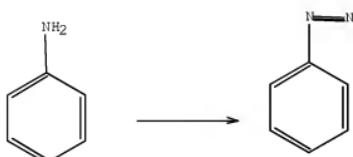
containing 11

L1 STRUCTURE UPLOADED

=> d L1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> file casreact  
COST IN U.S. DOLLARS  
FULL ESTIMATED COST

SINCE FILE ENTRY TOTAL  
SESSION  
0.46 0.67

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FILE CONTENT:1840 - 18 Oct 2008 VOL 149 ISS 17

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\*\*\*\*\*  
\*  
\* CASREACT now has more than 15.3 million reactions \*  
\*  
\*\*\*\*\*

CASREACT contains reactions from CAS and from: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s L1 SSS full  
FULL SEARCH INITIATED 10:01:17 FILE 'CASREACT'  
SCREENING COMPLETE - 22603 REACTIONS TO VERIFY FROM 2507 DOCUMENTS  
100.0% DONE 22603 VERIFIED 1129 HIT RXNS 177 DOCS  
SEARCH TIME: 00.00.05

L2 177 SEA SSS FUL L1 ( 1129 REACTIONS)

=> s L2 AND (diazonium salt)  
2459 DIAZONIUM  
52705 SALT  
886 DIAZONIUM SALT  
(DIAZONIUM(W)SALT)  
L3 15 L2 AND (DIAZONIUM SALT)

=> d ibib abs hitstr 1-  
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data

CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PATS ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN  
must be entered on the same line as DISPLAY, e.g.,  
D SCAN.)  
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
all single-step reactions)  
STD ----- BIB, IPC, and NCL  
  
CRD ----- Compact Display of All Hit Reactions  
CRDREF ----- Compact Reaction Display and SO, PY for Reference  
FHIT ----- Reaction Map, Diagram, and Summary for first  
hit reaction  
FHITCBIB --- FHIT, AN plus CBIB  
FCRD ----- First hit in Compact Reaction Display (CRD) format  
FCRDREF ----- First hit in Compact Reaction Display (CRD) format with  
CA reference information (SO, PY). (Default)  
FPATH ----- PATH, plus Reaction Summary for the "long path"  
FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
HIT ----- Reaction Map, Reaction Diagram, and Reaction  
Summary for all hit reactions and fields containing  
hit terms  
OCC ----- All hit fields and the number of occurrences of the  
hit terms in each field. Includes total number of  
HIT, PATH, SPATH reactions. Labels reactions that have  
incomplete verifications.  
PATH ----- Reaction Map and Reaction Diagram for the "long  
path". Displays all hit reactions, except those  
whose steps are totally included within another hit  
reaction which is displayed  
RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
RXS ----- Hit Reaction Summariers (Map and Summary for all hit reactions)  
SPATH ----- Reaction Map and Reaction Diagram for the "short  
path". Displays all single step reactions which  
contain a hit substance. Also displays those  
multistep reactions that have a hit substance in both  
the first and last steps of the reaction, except for  
those hit reactions whose steps are totally included  
within another hit reaction which is displayed

To display a particular field or fields, enter the display field  
codes. For a list of the display field codes, enter HELP DFIELDS  
at an arrow prompt (>). Examples of combinations include: D TI;

D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CCRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

(FILE 'HOME' ENTERED AT 10:00:42 ON 20 OCT 2008)

FILE 'REGISTRY' ENTERED AT 10:00:50 ON 20 OCT 2008  
L1 STRUCTURE uploaded

FILE 'CASREACT' ENTERED AT 10:01:12 ON 20 OCT 2008  
L2 177 S L1 SSS FULL  
L3 15 S L2 AND (DIAZONIUM SALT)

=> d ibib abs hitstr 1-  
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ABS ----- GI and AB  
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CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
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IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
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D SCAN.)  
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 OCC ----- All hit fields and the number of occurrences of the  
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 HIT, PATH, SPATH reactions. Labels reactions that have  
 incomplete verifications.  
 PATH ----- Reaction Map and Reaction Diagram for the "long  
 path". Displays all hit reactions, except those  
 whose steps are totally included within another hit  
 reaction which is displayed  
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
 RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
 RXS ----- Hit Reaction Summarizers (Map and Summary for all hit reactions)  
 SPATH ----- Reaction Map and Reaction Diagram for the "short  
 path". Displays all single step reactions which  
 contain a hit substance. Also displays those  
 multistep reactions that have a hit substance in both  
 the first and last steps of the reaction, except for  
 those hit reactions whose steps are totally included  
 within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

(FILE 'HOME' ENTERED AT 10:00:42 ON 20 OCT 2008)

FILE 'REGISTRY' ENTERED AT 10:00:50 ON 20 OCT 2008  
L1 STRUCTURE uploaded

FILE 'CASREACT' ENTERED AT 10:01:12 ON 20 OCT 2008  
L2 177 S L1 SSS FULL  
L3 15 S L2 AND (DIAZONIUM SALT)

=> s L3  
2459 DIAZONIUM  
52705 SALT  
886 DIAZONIUM SALT  
(DIAZONIUM(W) SALT)

=> d ibib abs hitstr 1-  
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

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CA reference information (SO, PY). (Default)  
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Summary for all hit reactions and fields containing  
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HIT, PATH, SPATH reactions. Labels reactions that have  
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RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
RXS ----- Hit Reaction Summariers (Map and Summary for all hit reactions)  
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contain a hit substance. Also displays those  
multistep reactions that have a hit substance in both  
the first and last steps of the reaction, except for  
those hit reactions whose steps are totally included  
within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CCRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

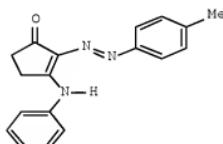
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FILE 'REGISTRY' ENTERED AT 10:00:50 ON 20 OCT 2008  
L1 STRUCTURE UPLOADED

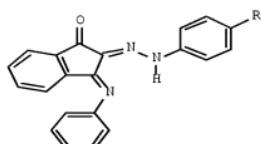
FILE 'CASREACT' ENTERED AT 10:01:12 ON 20 OCT 2008  
L2 177 S L1 SSS FULL  
L3 15 S L2 AND (DIAZONIUM SALT)  
L4 15 S L3

=> d ibib abs fhit

L4 ANSWER 1 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 147:72477 CASREACT Full-text  
TITLE: Synthesis and structure of some azo coupled cyclic  
β-enaminones  
AUTHOR(S): Simunek, Petr; Luskova, Lucie; Svobodova, Marketa;  
Bertolasi, Valerio; Lycka, Antonin; Machacek, Vladimir  
CORPORATE SOURCE: Department of Organic Chemistry, University of  
Pardubice, Pardubice, CZ-532 10, Czech Rep.  
SOURCE: Magnetic Resonance in Chemistry (2007), 45(4), 330-339  
CODEN: MRCHEG; ISSN: 0749-1581  
PUBLISHER: John Wiley & Sons Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



I

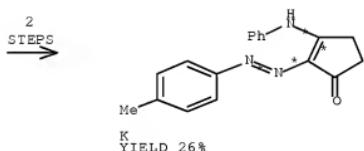
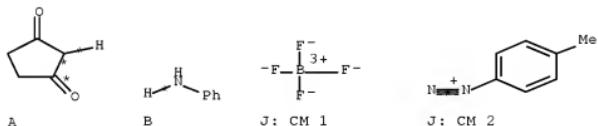


II

AB The reaction of 3-phenylaminocyclopent-2-en-1-one with 4-Me, 4-methoxy and 4-chlorobenzenediazonium tetrafluoroborates was used to prepare the azo coupling products, e.g., I. It was found that these compds. are present in both  $\text{CDCl}_3$  solution and solid phase practically exclusively as (E)-3-phenylamino-2-(4-

subst. phenyldiaz恒) cyclopent-2-en-1-ones with N-H...N intramol. hydrogen bond. The substitution of the Ph residue of the diazonium salt has no effect on the position of the tautomeric equilibrium. On the other hand, the compds. (II; R = Me or H) formed by the reaction of 3-phenylamino-1H-inden-1-one with 4-methylbenzene- or benzenediazonium tetrafluoroborates exist in  $\text{CDCl}_3$  solution and in solid phase as hydrazone compds. In the solution they occur as a mixture of three forms, out of which two were identified as E/Z isomers with different types of hydrogen bonds. The compound formed by the reaction of 3-amino-5,5-dimethylcyclohex-2-en-1-one with 4-methoxybenzenediazonium tetrafluoroborate is converted into a stable hydrochloride on standing in  $\text{CHCl}_3$  solution; this product exhibits a high degree of delocalization of the pos. charge. Its structure was studied by means of X-ray.

RX(9) OF 14 COMPOSED OF RX(1), RX(3)  
 RX(9) A + B + J ==> K



RX(1) RCT A 3859-41-4, B 62-53-3  
 PRO C 73825-35-1  
 SOL 108-88-3 PhMe  
 CON SUBSTAGE(1) 4 hours, reflux  
 SUBSTAGE(2) cooled

RX(3)	RCT	C 73825-35-1, J 459-44-9
	RGT	L 127-09-3 AcONa
	PRO	K 941717-55-1
	SOL	75-09-2 CH2Cl2
	CON	24 hours, room temperature
	NTE	stereoselective

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMATORY.

=> d ibib abs fhit 1-

YOU HAVE REQUESTED DATA FROM 15 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 147:72477 CASREACT Full-text

TITLE: Synthesis and structure of some azo coupled cyclic  
β-enaminones

AUTHOR(S): Simunek, Petr; Luskova, Lucie; Slobodova, Marketa;  
Bertolasi, Valerio; Lycka, Antonin; Machacek, Vladimir

CORPORATE SOURCE: Department of Organic Chemistry, University of  
Pardubice, Pardubice, CZ-532 10, Czech Rep.

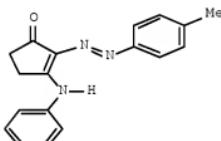
SOURCE: Magnetic Resonance in Chemistry (2007), 45(4), 330-339  
CODEN: MRCHEG; ISSN: 0749-1581

PUBLISHER: John Wiley & Sons Ltd.

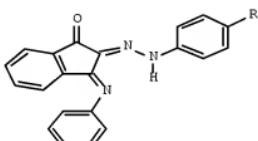
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



I

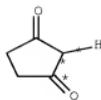


II

AB The reaction of 3-phenylaminocyclopent-2-en-1-one with 4-Me, 4-methoxy and 4-chlorobenzenediazonium tetrafluoroborates was used to prepare the azo coupling products, e.g., I. It was found that these compds. are present in both  $\text{CDCl}_3$  solution and solid phase practically exclusively as (E)-3-phenylamino-2-(4-subst. phenyldiazaryl)cyclopent-2-en-1-ones with N-H...N intramol. hydrogen bond. The substitution of the Ph residue of the diazonium salt has no effect on the position of the tautomeric equilibrium. On the other hand, the compds. (II; R = Me or H) formed by the reaction of 3-phenylamino-1H-inden-1-one with 4-methylbenzene- or benzenediazonium tetrafluoroborates exist in  $\text{CDCl}_3$  solution and in solid phase as hydrazone compds. In the solution they occur as a mixture of three forms, out of which two were identified as E/Z isomers with different types of hydrogen bonds. The compound formed by the reaction of 3-amino-5,5-dimethylcyclohex-2-en-1-one with 4-methoxybenzenediazonium tetrafluoroborate is converted into a stable hydrochloride on standing in  $\text{CHCl}_3$  solution; this product exhibits a high degree of delocalization of the pos. charge. Its structure was studied by means of X-ray.

RX(9) OF 14 COMPOSED OF RX(1), RX(3)

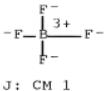
RX(9) A + B + J ==> K



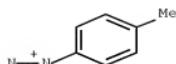
A



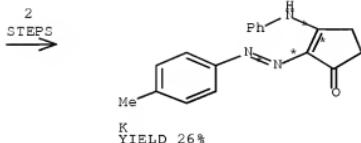
B



J: CM 1



J: CM 2



RX(1) RCT A 3859-41-4, B 62-53-3  
PRO C 73825-35-1  
SOL 108-88-3 PhMe  
CON SUBSTAGE(1) 4 hours, reflux  
SUBSTAGE(2) cooled

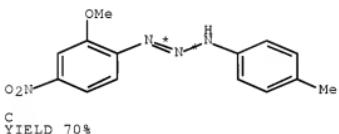
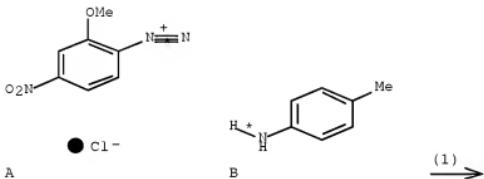
RX(3) RCT C 73825-35-1, J 459-44-9  
RGT L 127-09-3 AcONa  
PRO K 941717-55-1  
SOL 75-09-2 CH<sub>2</sub>C<sub>12</sub>  
CON 24 hours, room temperature  
NTE stereoselective  
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 143:459818 CASREACT [Full-text](#)  
TITLE: 2-Methoxy-4-nitrobenzenediazonium salt as a practical diazonium-transfer agent for primary arylamines via tautomerism of 1,3-diaryltriazenes: Deaminative iodination and arylation of arylamines without direct diazotization

AUTHOR(S): Saeki, Tomoyuki; Son, Eun-Cheol; Tamao, Kohei  
CORPORATE SOURCE: International Research Center for Elements Science, Institute for Chemical Research, Kyoto University, Uji, Japan  
SOURCE: Bulletin of the Chemical Society of Japan (2005), 78(9), 1654-1658  
PUBLISHER: Chemical Society of Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB 1,3-Diaryltriazenes, prepared from a 2-methoxy-4-nitrobenzenediazonium salt and primary arylamines, exist as azo-transfer tautomers in which the 2-methoxy-4-nitrophenyl group is present on the saturated nitrogen atom and forms a hydrogen bond between the 2-methoxy group and the N-H moiety. The synthetic utility of the diazonium salt as a practical diazonium-transfer agent for primary arylamines via tautomerism of the 1,3-diaryltriazenes has been demonstrated by the deaminative iodination and arylation of the arylamines without direct diazotization. The starting 2-methoxy-4-nitrophenylamine can be easily recovered after the reactions.

RX(1) OF 37 A + B ==> C...



RX(1) RCT A 120-17-2, B 106-49-0  
 RGT D 584-08-7 K2CO3  
 PRO C 869373-61-5  
 CON 30 minutes, 0 deg C

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 143:440299 CASREACT Full-text  
 TITLE: Studies with functionally substituted enamines: synthesis of new aminoazolo-pyrimidines and -1,2,4-triazines  
 AUTHOR(S): Ghozlan, Said Ahmed Soliman; Abdelhamid, Ismail  
 Abdelsahfy; Gaber, Hatem; Elnagdi, Mohamed Hilmy  
 CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Cairo University, Giza, Egypt

SOURCE:

Journal of Chemical Research (2004), (12), 789-793

PUBLISHER:

CODEN: JCROA4

DOCUMENT TYPE:

Science Reviews

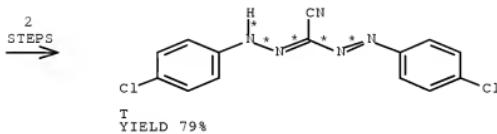
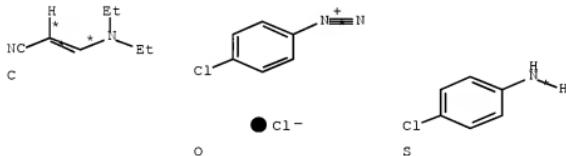
LANGUAGE:

Journal

AB 3-Aminocrylonitrile derivs., R1R2NCH:CHCN (R1 = R2 = Et (1d), Ph (1e), (CH2)5 (1f), (CH2CH2)2O (1g)) coupled with aromatic and heteroarom. diazonium salts yielding arylhydrazons and pyrazolo[5,1-c]triazines. The enaminonitriles 1 condensed to form dienes on reflux in acetic acid. The latter underwent Diels-Alder type addition to naphthoquinone. Aminopyrazolopyrimidines were obtained from reaction of 1d-1g with heteroarom. aminoazoles. Enaminonitrile 1d formed pyran with benzylidene malononitrile, and dihydropyrimidine with benzaldehyde and urea.

RX(47) OF 57 COMPOSED OF RX(6), RX(8)

RX(47) C + O + S ==&gt; T



RX(6) RCT C 58243-06-4, O 2928-74-2

RGT M 127-09-3 AcONa

PRO P 849820-80-0

SOL 64-19-7 AcOH

CON 1 hour, room temperature

RX(8) RCT S 106-47-8

STAGE(1)

RGT U 7647-01-0 HCl, V 7632-00-0 NaNO2

SOL 7732-18-5 Water

CON room temperature

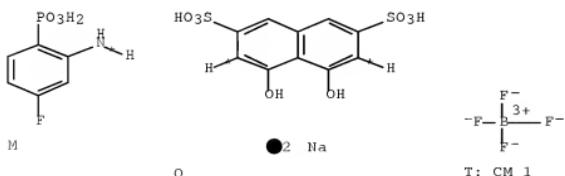
STAGE (2)  
 RCT P 849820-80-0  
 RGT M 127-09-3 AcONa  
 SOL 64-17-5 EtOH  
 CON room temperature

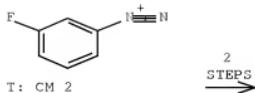
PRO T 7071-45-6  
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 143:286545 CASREACT Full-text  
TITLE: Synthesis of fluorophosphonoazo derivative as color  
reagent for thorium  
INVENTOR(S): Wu, Bincai; Wang, Bing  
PATENT ASSIGNEE(S): East China Normal University, Peop. Rep. China  
SOURCE: Faming Zhanli Shenqing Gongkai Shuomingshu, 9 pp.  
CODEN: CNXXEV  
DOCUMENT TYPE: Patent  
LANGUAGE: Chinese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

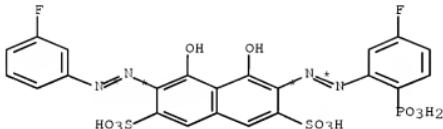
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1450071	A	20031022	CN 2003-116907	20030514
PRIORITY APPLN. INFO.:			CN 2003-116907	20030514
AB	The title compound, 2-(5-fluoro-2-phosphonophenylazo)-7-(3-fluorophenylazo)-1,8-dihydroxy-3,6-naphthalenedisulfonic acid, is synthesized by nitrifying 4-fluoroaniline with fuming HNO <sub>3</sub> /glacial acetic acid in glacial acetic acid/acetic anhydride to obtain 4-fluoro-2-nitroaniline, diazotizing with NaNO <sub>2</sub> in HCl solution and then salifying with NaBF <sub>4</sub> , reducing and substituting with PCl <sub>3</sub> in Et acetate in the presence of CuCl, hydrolyzing with water to obtain 2-amino-4-fluorophenylphosphonic acid, diazotizing, coupling with chromotropic acid Na salt, and then coupling with diazonium salt of 4-fluoroaniline. Th(IV) is determined by spectrophotometry at 680 nm in 6M HCl medium with m-fluoroazofluorophosphine as color developing agent and 1-butanol as extractant.			

RX(9) OF 15 COMPOSED OF RX(4), RX(5)  
RX(9) M + O + T ==> II





2  
STEPS



U

RX(4) RCT M 648863-06-9

STAGE(1)  
 RGT I 7632-00-0 NaNO<sub>2</sub>, J 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON 0.5 hours, 0 deg C

STAGE(2)  
 RCT Q 129-96-4  
 RGT S 127-09-3 AcONa  
 SOL 7732-18-5 Water  
 CON 1 hour, 10 deg C

STAGE(3)  
 RGT J 7647-01-0 HCl  
 SOL 7732-18-5 Water  
 CON pH <1

PRO R 681145-02-8

RX(5) RCT R 681145-02-8, T 1996-38-9

STAGE(1)  
 RGT V 1310-65-2 LiOH  
 SOL 7732-18-5 Water  
 CON 1 hour, 0 deg C, pH 8 - 10

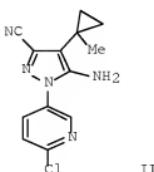
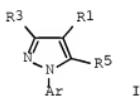
STAGE(2)  
 RGT W 12408-02-5 H+  
 SOL 7732-18-5 Water

PRO U 864380-51-8

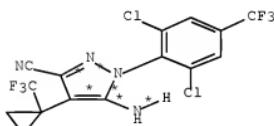
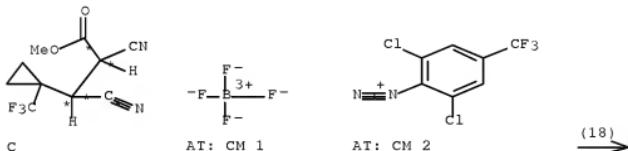
L4 ANSWER 5 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 142:316832 CASREACT Full-text  
TITLE: Process for the preparation of substituted aryl  
pyrazoles via cyclization of diazo compounds with  
2,3-dicyanopropionates and related derivatives  
INVENTOR(S): Gladwell, Iain Robert; Matthews, John George; Pettman,  
Alan John  
PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.  
SOURCE: PCT Int. Appl., 69 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005023773	A1	20050317	WO 2004-IB2758	20040824
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20050096354	A1	20050505	US 2004-932390	20040902
PRIORITY APPLN. INFO.:			GE 2003-20719	20030904
			GB 2004-14893	20040702
			US 2003-517349P	20031104
			US 2004-600405P	20040809

OTHER SOURCE(S): MARPAT 142:316832  
GI



AB The invention is related to a process for the preparation of the well-known pesticides aminocyno 1-arylpyrazoles and 1-pyridinylpyrazoles of formula I via cyclization of aryl diazonium compds. Ar-N<sup>+</sup>.tblond.BNX- (prepared in situ or isolated) with compds. of formula R3LCH-CHR1R5a, e.g. alkyl 2,3-dicyanopropionates, optionally in the presence of an acid [Ar = (un)substituted Ph, pyridinyl; R1 = (un)substituted alkyl, cycloalkyl, 5- or 6-membered heterocycl, cyclopropyl, fused bicyclic, etc.; R3 = CN, CF<sub>3</sub>, CHO, COR, CO2R; R = (un)substituted alkyl; R5 = H, (un)substituted alkyl; R5a = CN, CO2H, CHO, COR; CO2R; L = activating group; X = compatible counter ion]. The advantages include improved product yield, lower reaction time, and reduced number of steps. Thus, reacting Me 2,3-dicyano-3-(1-methylcyclopropyl)propanoate (preparation given) with 6-chloropyridine-3-diazonium•BF<sub>4</sub><sup>-</sup> (preparation given) in MeCN at 0° for 20 min and at room temperature for 3 h, followed by treatment of the reaction mixture with NH4OH gave pyrazole II in 68% yield.



AU  
YIELD 31%

RX(18) RCT C 848074-26-0, AT 258353-28-5  
 RGT AY 127-09-3 AcONa  
 PRO AU 208937-91-1  
 SOL 67-56-1 MeOH  
 CON SUBSTAGE(1) room temperature  
           SUBSTAGE(2) 15 minutes, cooled  
           SUBSTAGE(3) 4.5 hours, room temperature  
 NTE NaHCO<sub>3</sub> can also be used as base, sonication before the addition

of diazonium salt

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 139:360542 CASREACT Full-text

TITLE: Photochemical DNA cleavage by a Berenil analog

AUTHOR(S): Burr, Sally J.; Mselati, Abdulghani; Thomas, Emrys W.

CORPORATE SOURCE: Division of Biological Sciences, Salford University, Salford, M5 4WT, UK

SOURCE: Tetrahedron Letters (2003), 44(39), 7307-7309

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science B.V.

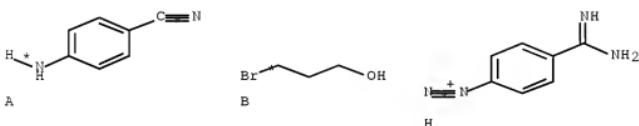
DOCUMENT TYPE: Journal

LANGUAGE: English

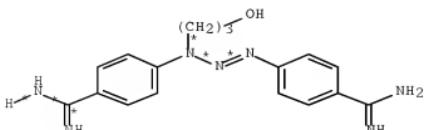
AB Berenil [bis(4-amidinophenyl)1,3-triazene] is a photostable DNA-binding ligand. We describe here the synthesis of N-(3-hydroxypropyl)-Berenil, which in contrast to Berenil is photosensitive to 360 nm irradiation, behaving as a caged diazonium salt. The 4-amidinobenzene diazonium fragment produced by photolysis induces DNA modification and cleavage.

RX(6) OF 6 COMPOSED OF RX(1), RX(2), RX(3)

RX(6) A + B + H ==> I



3  
STEPS  
→



I  
YIELD 50%

RX(1) RCT A 673-74-5, B 627-18-9  
PRO C 313238-55-0  
NTE no exptl. details

RX(2) RCT C 313238-55-0

STAGE(1)  
RGT E 7647-01-0 HCl  
SOL 67-56-1 MeOH

STAGE(2)  
RGT F 7664-41-7 NH3  
SOL 67-56-1 MeOH

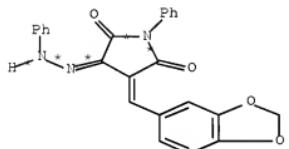
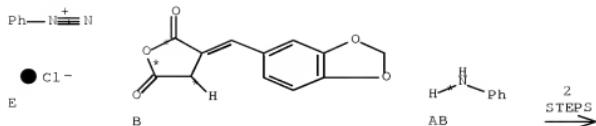
PRO D 620947-05-9

RX(3) RCT D 620947-05-9, H 620947-06-0  
PRO I 620947-07-1  
NTE no exptl. details

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 139:214429 CASREACT Full-text  
TITLE: Synthesis of azo-coupled etaconic acid anhydride and its reactions with nucleophiles  
AUTHOR(S): Prabhu, P. J.; Bhise, N. B.; Dave, M. A.  
CORPORATE SOURCE: Department of Chemistry, K.J. Somaiya College of Science and Commerce, Mumbai, 400 077, India  
SOURCE: Asian Journal of Chemistry (2003), 15(2), 634-638  
CODEN: AJCHEW; ISSN: 0970-7077  
PUBLISHER: Asian Journal of Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB 3,4-Methylenedioxy-benzylidene succinic anhydride was condensed with diazonium salts of various aromatic amines to form hydrazones or dyes which were further treated with nucleophiles like 10% NaOH and NaBH4 to give various pyrazolinone derivs., resp. and cyclic imide derivs. of the corresponding hydrazones. The antibacterial and antifungal activities of some the products are also reported.

RX(24) OF 45 COMPOSED OF RX(2), RX(14)  
RX(24) E + B + AB ==> AC



AC  
YIELD 64%

RX(2) RCT E 100-34-5

STAGE(1)  
RGT G 7647-01-0 HCl, H 7632-00-0 NaNO2  
SOL 7732-18-5 Water  
CON 15 minutes, 0 deg C

STAGE(2)  
RCT B 99971-42-3  
SOL 67-64-1 Me2CO  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 30 minutes, 0 deg C

PRO F 587881-56-9

RX(14) RCT F 587881-56-9, AB 62-53-3

STAGE(1)  
SOL 64-17-5 EtOH  
CON 4 - 5 hours, reflux

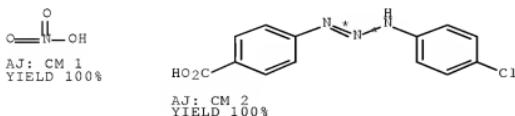
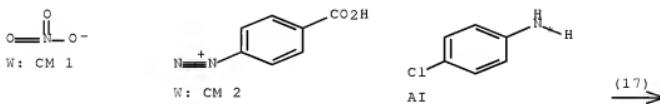
STAGE(2)  
CAT 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO AC 587881-78-5

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 137:124905 CASREACT Full-text  
 TITLE: Waste-free chemistry of diazonium salts and benign separation of coupling products in solid salt reactions  
 AUTHOR(S): Kaupp, Gerd; Herrmann, Andreas; Schmeyers, Jens  
 CORPORATE SOURCE: Universitat Oldenburg FB Chemie, Organische Chemie I, Oldenburg, 26111, Germany  
 SOURCE: Chemistry--A European Journal (2002), 8(6), 1395-1406  
 PUBLISHER: Wiley-VCH Verlag GmbH  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Gas-solid and solid-solid techniques allow for waste-free and quant. syntheses in the chemical of diazonium salts. Five techniques for diazotations with the reactive gases NO<sub>2</sub>, NO and NOCl are studied. Two types are mechanistically investigated with atomic force microscopy (AFM) and are interpreted on the basis of known crystal packings. The same principles apply to the cascade reactions that had been derived from one-step reactions. Solid diazonium salts couple quant. with solid diphenylamine and anilines to give the triazenes. Azo couplings are achieved with quant. yields by cautious co-grinding of solid diazonium salts with  $\beta$ -naphthol and C-H acidic heterocycles, such as barbituric acids or pyrazolinones. Solid diazonium salts may be more easily applied in a stoichiometric ratio for couplings in solution. Co-grinding of solid diazonium salts with KI gives quant. yields of various solid aryl iodides. The unavoidable coupling products in salt reactions are completely separated from the insol. products in a highly benign manner. The solid-state reactions compare favorably with similar solution reactions that produce much waste. The structures of the products are elucidated with IR and NMR spectroscopy and mass spectrometry, while the tautomeric properties of the compds. are studied with d. functional calcns. at the B3LYP/6-31G\* and BLYP/6-31G\*\* levels. Safety: care must be taken when handling solid diazonium salts.

RX(17) OF 51      W + AI ==> AJ...



RX(17) RCT W 178412-89-0, AI 106-47-8

PRO AJ 444288-67-9

NTE solid state, green chem.

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 15 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 136:37382 CASREACT Full-text

TITLE: Reactions of diazonium salts with phenyl dithiocarbamate. Part II. Formation of related arylazophenyldithiocarbamates

AUTHOR(S): Haque, M. Zahurul; Ali, M. Umar; Ali, M. Hossen

CORPORATE SOURCE: BCSIR Laboratories, Rajshahi, Bangladesh

SOURCE: Journal of the Indian Chemical Society (2001), 78(7), 372-373

CODEN: JICSAH; ISSN: 0019-4522

PUBLISHER: Indian Chemical Society

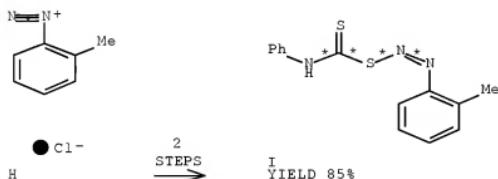
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Reaction of 1-naphthyl diazonium salt with ammonium salt of phenyldithiocarbamic acid gives 1-naphthylazophenyldithiocarbamate. Similar reaction has been carried out with several other aryl diazonium chlorides. Antibacterial activity of the compds. has been evaluated.

RX(10) OF 15 COMPOSED OF RX(1), RX(3)

RX(10) A + B + H ==> I



RX(1) RCT A 75-15-0, B 62-53-3

RG D 1336-21-6 NH4OH

PRO C 1074-52-8

SOL 7732-18-5 Water

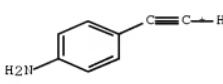
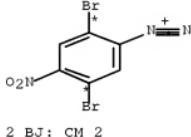
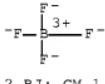
RX(3) RCT C 1074-52-8, H 2028-34-4

PRO I 380149-05-3  
SOL 7732-18-5 Water

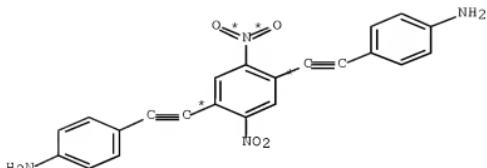
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 134:353093 CASREACT Full-text  
TITLE: Phenylene ethynylene diazonium salts as potential self-assembling molecular devices  
AUTHOR(S): Kosynkin, Dmitry V.; Tour, James M.  
CORPORATE SOURCE: Department of Chemistry and Center for Nanoscale Science and Technology, Rice University, Houston, TX, 77005, USA  
SOURCE: Organic Letters (2001), 3(7), 993-995  
CODEN: ORLEF7; ISSN: 1523-7060  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Functionalized diazonium salts for mol. electronic devices are prepared by the reaction of the corresponding anilines with  $\text{NOBF}_4$  in sulfolane-MeCN solvent.

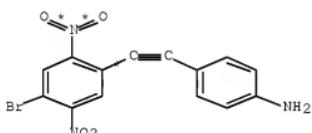
RX(48) OF 133 COMPOSED OF RX(26), RX(1)  
RX(48) 2 BJ + 3 B ==> C + D



2  
STEPS  
→



C  
YIELD 36%



D  
YIELD 43%

RX(26) RCT BJ 339175-69-8  
RGT BK 7632-00-0 NaNO<sub>2</sub>  
PRO A 18908-08-2  
SOL 7732-18-5 Water

RX(1) RCT A 18908-08-2, B 14235-81-5  
RGT E 121-44-8 Et<sub>3</sub>N  
PRO C 339175-50-7, D 339175-70-1  
CAT 13965-03-2 PdCl<sub>2</sub>(PPh<sub>3</sub>)<sub>2</sub>, 7681-65-4 CuI  
SOL 109-99-9 THF

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 130:168232 CASREACT Full-text

TITLE: Preparation of O-(perfluoroalkyl)dibenzofuranium salts as perfluoroalkylating agents and their intermediates such as (perfluoroalkoxy)biphenyldiazonium salts

INVENTOR(S): Umemoto, Teruo; Adachi, Kenji; Ishihara, Sumi

PATENT ASSIGNEE(S): Daikin Industries Ltd., Japan

SOURCE: PCT Int. Appl., 49 pp.

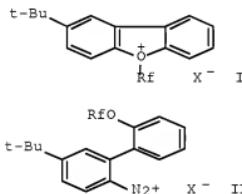
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

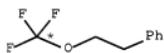
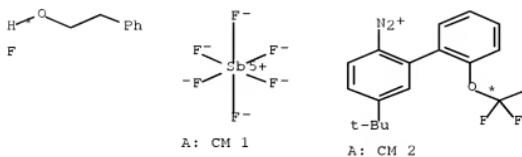
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906389	A1	19990211	WO 1998-JP3416	19980730
W: JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1013651	A1	20000628	EP 1998-935301	19980730
EP 1013651	B1	20070530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 363477	T	20070615	AT 1998-935301	19980730
US 6239289	B1	20010529	US 2000-463706	20000215
PRIORITY APPLN. INFO.:			JP 1997-207901	19970801
			WO 1998-JP3416	19980730
OTHER SOURCE(S):	MARPAT 130:168232			
GI				



AB O-(Perfluoroalkyl)dibenzofuran salt derivs. represented by general formula (I; Rf is perfluoroalkyl being 1 to 10 carbon atoms; and X- is a conjugate base of a Bronsted acid) are prepared by cyclization of (perfluoroalkoxy)diphenyl diazonium salts (II; RF and X- are defined as above) and are used as perfluoroalkylating agents for perfluoroalkylation of nucleophiles containing O or N, e.g. amines and alcs. When the O-(perfluoroalkyl)dibenzofuran salt derivs. are used as perfluoroalkylating agents, they permit high-yield perfluoroalkylation, and are applicable to a wide range of compds. and inhibited in self-decomposition as to be relatively stable. The presence of tert-Bu at 5-position improves the stability of I and thereby usefulness of I as perfluoroalkylating agents. Thus, a solution of 7.17 g 2-amino-5-tert-butyl-2'-(trifluoromethoxy)biphenyl in 46 mL Et2O was cooled to -78° with stirring, followed by adding 6.47 g nitrosonium hexafluoroantimonate (ON+SbF6-), and the resulting mixture was warmed to 10° over 3 h in a warm bath, while adding 10 mL Et2O when temperature reached to 5°, to give 58% II (Rf = CF3, X- = SbF6-) (III). A CCl2D2 solution of 6.5 mg III in a Pyrex NMR tube was cooled to -106° and irradiated by a high pressure Hg lamp (400 W and 253.7 nm) for 45 min to give I (Rf = CF3, X- = SbF6-) (IV) 87, 5-tert-butyl-2-fluoro-2'-(trifluoromethoxy)biphenyl 8, and 5-tert-butyl-2-chloro-2'-(trifluoromethoxy)biphenyl 3% according to 19F- and 1H-NMR anal. at -80°. When the temperature was gradually raised to -30°, IV completely decomposed to CF4 and 2-tert-butylbenzofuran. To the cold (-99° to -90°) reaction mixture similarly prepared were added variety of alcs. and amines. When phenecyl alc. was added at -90°, the resulting mixture was warmed to -10° over 3 h to give 80% phenecyl trifluoromethyl ether. Although in general, diazonium salts are explosive in nature, III has .apprx.27° higher

decomposition temperature (84.7–85.8°) compared to that of the 4-tert-Bu regioisomer (m.p. 58–60°) and can be handled at room temperature, and safely stored and transported.



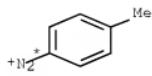
<sup>G</sup>  
YIELD 70%

RX(2) RCT F 60-12-8, A 220351-08-6  
 PRO G 175676-47-8  
 SOL 75-09-2 CH2C12  
 NTE two-step reaction involving in situ prepn. of  
 O-(trifluoromethyl)dibenzofuranium salt under irradn. of  
 (trifluoromethoxy)debenzofuran-2-diazonium  
 salt with a high pressure Hg lamp at -99° to  
 -90° for 70 min followed by trifluoromethylation at  
 -90° to -10° for 3 h  
 REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. 0 CITATIONS AVAILABLE IN THE RE FORMAT

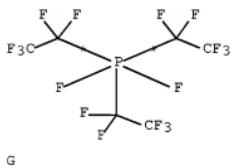
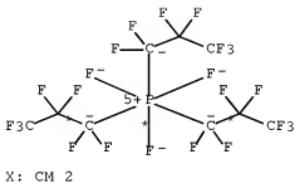
L4 ANSWER 12 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 111:174247 CASREACT [Full-text](#)  
 TITLE: Reaction of tris(perfluoroalkyl)phosphine oxides and  
 tris(perfluoroalkyl)difluorophosphoranes with fluoride  
 ion  
 AUTHOR(S): Pavlenko, N. V.; Yagupol'skii, L. M.  
 CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR  
 SOURCE: Zhurnal Obshchei Khimii (1989), 59(3), 528-34  
 DOCUMENT TYPE: CODEN: ZOKHA4; ISSN: 0044-460X  
 LANGUAGE: Journal  
 Russian  
 AB Treating (C2F5)3P(O) with 1 or 2 equivalent CsF in Et2O gave (C2F5)3PF5Cs or  
 (C2F5)2PF2OCs, resp.; hydrolysis of the latter gave C2F5P(O)FOCs. Treating  
 R3PF2 (R = C2F5, C3F7, C4F9) with MF (M = Cs, K, Na) in Et2O gave quant.

$\text{M} + [\text{R}_3\text{PF}_3]^-$ . Diazotization of  $4-\text{X-C}_6\text{H}_4\text{NH}_2$  ( $\text{X} = \text{Cl, Me, NO}_2$ ) and subsequent reaction with  $\text{K}^+[\text{R}_3\text{PF}_3]^-$  ( $\text{R} = \text{C}_2\text{F}_5, \text{C}_3\text{F}_7$ ) gave 77-88%  $[4-\text{X-C}_6\text{H}_4\text{N}_2]^+[\text{R}_3\text{PF}_3]^-$ .

$\text{RX(40) OF 63 COMPOSED OF RX(11), RX(7), RX(10), RX(18)}$   
 $\text{RX(40)} \quad \text{X} + \text{T} \implies \text{S} + \text{G}$



X: CM 1



RX(11) RCT X 123199-73-5  
 PRO Y 352-32-9, M 91543-33-8  
 NTE thermal

RX(7) RCT M 91543-33-8  
 RGT J 7789-23-3 KF  
 PRO O 123199-67-7  
 SOL 60-29-7 Et2O

RX(10) RCT T 106-47-8

STAGE(1)

RGT V 7647-01-0 HCl, W 7632-00-0 NaNO2  
SOL 7732-18-5 Water

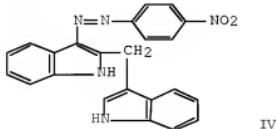
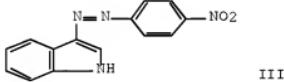
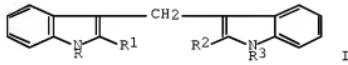
STAGE(2)

RCT O 123199-67-7  
SOL 7732-18-5 Water

PRO U 123199-72-4

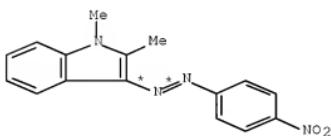
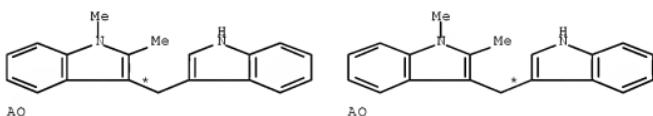
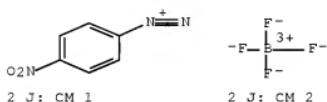
RX(18) RCT U 123199-72-4  
PRO S 352-33-0, G 91543-32-7  
NTE thermal

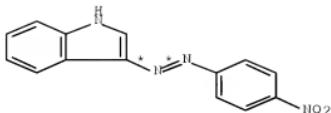
L4 ANSWER 13 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 108:221504 CASREACT Full-text  
TITLE: Electrophilic substitution in indoles. Part 15. The reaction between methylenediindoles and p-nitrobenzenediazonium fluoroborate  
AUTHOR(S): Jackson, Anthony H.; Prasitpan, Noojaree; Shannon, Patrick V. R.; Tinker, Alan C.  
CORPORATE SOURCE: Dep. Chem., Univ. Coll., Cardiff, CF1 1XL, UK  
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1987), (11), 2543-51  
CODEN: JCPRB4; ISSN: 0300-922X  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB The preparation and substitution reaction of methylene diindoles I (R-R3 = H; R = R3 = Me, R1 = R2 = H; R = R1 = H, R2 = R3 = Me; R = R2 = R3 = H, R1 = Me)

with 4-O2NC6H4N2+ BF4- (II) are described. Thus, indole was treated with aqueous CH2O in AcOH to give 98% I (R=R3 = H). Reacting the latter I with II in MeCN gave a mixture of 45% (nitrophenylazo)indole III and 39% methylenedindiindole IV. The displacement of indolylmethyl residues from methylenedindiindoles by II, and the formation of the azo coupled rearrangement product IV provides evidence that azo coupling of 3-alkylindoles to give 2,3-disubstituted indoles proceeds by initial attack at the 3-position followed by rearrangement, rather than by direct substitution at the 2-position.

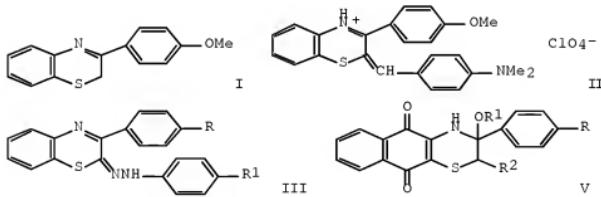




Y

RX(26) RCT J 456-27-9, AQ 114648-74-7  
 PRO S 114648-69-0, Y 53330-79-3  
 SOL 64-17-5 EtOH, 7732-18-5 Water  
 NTE 2 equiv. diazonium salt

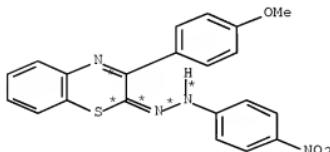
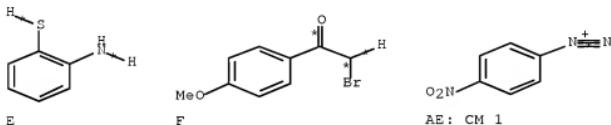
L4 ANSWER 14 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 94:48807 CASREACT Full-text  
 TITLE: New dyes based on 3-arylbenzo- and  
 -naphtho-1,4-thiazines  
 AUTHOR(S): MacKenzie, Neil E.; Thomson, Ronald H.; Greenhalgh,  
 Colin W.  
 CORPORATE SOURCE: Dep. Chem., Univ. Aberdeen, Aberdeen, AB9 2UE, UK  
 SOURCE: Journal of the Chemical Society, Perkin Transactions  
 1: Organic and Bio-Organic Chemistry (1972-1999)  
 (1980), (12), 2923-32  
 CODEN: JCPRB4; ISSN: 0300-922X  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB 3-Aryl-2H-1,4-benzothiazines were converted into cyanine dyes by condensing their perchlorates with aldehydes, and into azo compds. by coupling with reactive diazonium salts. E.g., condensation of the perchlorate [76149-00-3] of benzothiazine I with 4-Me2NC6H4CHO [100-10-7] gave 70% blue perchlorate II [76149-01-4], the free base of which was orange, whereas I [76148-93-1] coupled with 4-MeO2CC6H4N2+SO4- [76148-96-4] to give 65% azo dye III (R = OMe, R1 = CO2Me) [76148-95-3]. The azo compds. were also obtained by

condensing arylglyoxal hydrazone bromides with 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>SnNa [52380-58-2]. E.g., PhCOCB<sub>r</sub>:NNHPh [55716-62-6] condensed with 2-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>SnNa to give 84% III (R = R<sub>1</sub> = H) [76148-94-2]. 2-Amino-3-mercapto-1,4-naphthoquinone (IV) [76148-76-0] condensed with  $\alpha$ -bromoacetophenones to give naphthothiazinequinones. E.g., IV with BrCH<sub>2</sub>COC<sub>6</sub>H<sub>4</sub>OMe-4 [2632-13-5] gave 95% naphthothiazinequinone V (R = OMe, R<sub>1</sub> = R<sub>2</sub> = H) [76148-98-6]. Attempts to dehydrate the naphthothiazinequinones gave a variety of products; reactions included extrusion of S and loss of H<sub>2</sub>O giving indolequinones and oxidative dimerization of the quinones. Oxidation of V (R = R<sub>1</sub> = R<sub>2</sub> = H) [76148-97-5] with iodosobenzene diacetate [3240-34-4] in AcOH gave 45% V (R = H, R<sub>1</sub> = Et, R<sub>2</sub> = OAc) [76148-99-7] by an indirect Pummerer oxidation

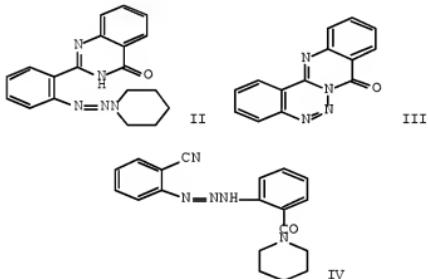
RX(46) OF 68 COMPOSED OF RX(2), RX(16)  
 RX(46) E + F + AE ==> AF



RX(2) RCT E 137-07-5, F 2632-13-5  
 PRO A 76148-93-1  
 CAT 141-52-6 NaOEt

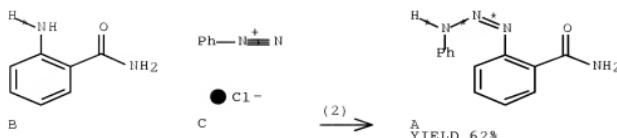
RX(16) RCT A 76148-93-1, AE 51979-06-7  
PRO AF 76148-69-1  
CAT 127-09-3 AcONa

L4 ANSWER 15 OF 15 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 84:180173 CASREACT [Full-text](#)  
TITLE: Approaches to the synthesis of  
quinazolino[1,2,3]benzotriazinones  
AUTHOR(S): Ahern, T. Patrick; Fong, Handrick; Vaughan, Keith  
CORPORATE SOURCE: Dep. Chem., St. Mary's Univ., Halifax, NS, Can.  
SOURCE: Canadian Journal of Chemistry (1976), 54(2), 290-6  
DOCUMENT TYPE: CODEN: CJCHAG; ISSN: 0008-4042  
LANGUAGE: Journal  
GI English



AB The 1-(o-carboxamidophenyl)-3-aryltriazenes o-RCOC<sub>6</sub>H<sub>4</sub>N:NNHC<sub>6</sub>H<sub>4</sub>R1-o I (R = NH<sub>2</sub>, R1 = H, CONH<sub>2</sub>; R = MeO, R1 = CONH<sub>2</sub>) were prepared from o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONH<sub>2</sub> and o-R1C<sub>6</sub>H<sub>4</sub>N<sub>2</sub><sup>+</sup> and reaction of o-MeO<sub>2</sub>CC<sub>6</sub>H<sub>4</sub>N<sub>2</sub><sup>+</sup> with o-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CO<sub>2</sub>NH<sub>2</sub>. Reaction of I (R = MeO, R1 = H<sub>2</sub>NCO) with piperidine in EtOH gave 2-[2-(piperidin-1-ylazo)phenyl]quinazolin-4(3H)-one (II). Quinazolino[3,2-c][1,2,3]benzotriazin-8-one (III) was obtained from IV by cyclization, rearrangement, and further cyclization.

RX(2) OF 7 B + C ==> A



RX(2) RCT B 88-69-6, C 100-34-5  
PRO A 59255-02-6

=> d his

(FILE 'HOME' ENTERED AT 10:00:42 ON 20 OCT 2008)

FILE 'REGISTRY' ENTERED AT 10:00:50 ON 20 OCT 2008  
L1 STRUCTURE UPLOADED

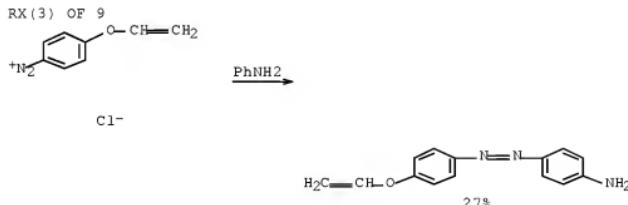
FILE 'CASREACT' ENTERED AT 10:01:12 ON 20 OCT 2008  
L2 177 S L1 SSS FULL  
L3 15 S L2 AND (DIAZONIUM SALT)  
L4 15 S L3

=> s L2 AND (nucleophil?)  
28295 NUCLEOPHIL?  
L5 13 L2 AND (NUCLEOPHIL?)

=> d scan

L5 13 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI (Vinylloxy)benzenediazonium chloride in reactions of nitrogen coupling and the exchange of the diazo group with nucleophilic reagents

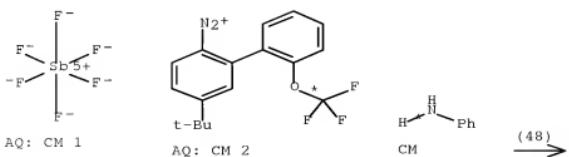


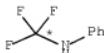
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d ibib abs fhit 1-  
YOU HAVE REQUESTED DATA FROM 13 ANSWERS - CONTINUE? Y/(N):y

L5 ANSWER 1 OF 13 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 147:406619 CASREACT Full-text  
 TITLE: CF<sub>3</sub> Oxonium Salts, O-(Trifluoromethyl)dibenzofuranium Salts: In Situ Synthesis, Properties, and Application as a Real CF<sub>3</sub><sup>+</sup> Species Reagent  
 AUTHOR(S): Umemoto, Teruo; Adachi, Kenji; Ishihara, Sumi  
 CORPORATE SOURCE: MEC Laboratory, Daikin Industries Ltd., Ibaraki, 305, Japan  
 SOURCE: Journal of Organic Chemistry (2007), 72(18), 6905-6917  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB We report in situ synthesis of the first CF<sub>3</sub> oxonium salts, thermally unstable O-(trifluoromethyl)dibenzofuranium salts, which furthermore have different counteranions (BF<sub>4</sub><sup>-</sup>, PF<sub>6</sub><sup>-</sup>, SbF<sub>6</sub><sup>-</sup>, and Sb<sub>2</sub>F<sub>11</sub><sup>-</sup>) and ring substituents (tert-Bu, F, and OCH<sub>3</sub>), by photochem. decomposition of the corresponding 2-(trifluoromethoxy)biphenyl-2'-diazonium salts at -90° to -100°. The yields markedly increased in the order of BF<sub>4</sub><sup>-</sup> < PF<sub>6</sub><sup>-</sup> < SbF<sub>6</sub><sup>-</sup> < Sb<sub>2</sub>F<sub>11</sub><sup>-</sup>. The CF<sub>3</sub> oxonium salts were fully assigned by means of <sup>1</sup>H and <sup>19</sup>F NMR spectroscopy at low temperature. The CF<sub>3</sub> salts decomposed to form CF<sub>4</sub> and dibenzofurans. The half-life times at -60° of the C-2 tert-Bu substituted salts having different counteranions were 29 min for the BF<sub>4</sub><sup>-</sup> salt, 36 min for the PF<sub>6</sub><sup>-</sup> salt, 270 min for the SbF<sub>6</sub><sup>-</sup> salt, and 415 min for the Sb<sub>2</sub>F<sub>11</sub><sup>-</sup> salt. Half-life times at -60° for Sb<sub>2</sub>F<sub>11</sub><sup>-</sup> salts having different C-2 substituents were 13 min for the fluoro C-2 substituted salt, 63 min for the unsubstituted salt, and 415 min for the tert-Bu C-2 substituted salt. Thus, the stability of the CF<sub>3</sub> oxonium salts increased in the counterion order of BF<sub>4</sub><sup>-</sup> < PF<sub>6</sub><sup>-</sup> < SbF<sub>6</sub><sup>-</sup> < Sb<sub>2</sub>F<sub>11</sub><sup>-</sup> and increased in the C-2 substituent order F < H < tert-Bu, which is in accord with the increasing non-nucleophilicity of counteranions and the electron-donating effect of ring substituents. 2-Tert-Butyl-O-(trifluoromethyl)dibenzofuranium hexafluoroantimonate was successfully applied as a CF<sub>3</sub><sup>+</sup> species source to the direct O- and N-trifluoromethylations of alcs., phenols, amines, anilines, and pyridines under very mild conditions. Thermal decomposition of a mixture of 2-[2-(F<sub>3</sub>C)C<sub>6</sub>H<sub>4</sub>N<sub>2</sub><sup>+</sup>]C<sub>6</sub>H<sub>4</sub>N<sub>2</sub><sup>+</sup> F<sub>6</sub>Sb<sup>-</sup> and aryl- or alkylsulfonic acids, pyridine, or pyridines having an electron-withdrawing group gave CF<sub>3</sub>O or CF<sub>3</sub>N products. The trifluoromethylation mechanism is discussed and an SN<sub>2</sub> mechanism containing the transient formation of free CF<sub>3</sub><sup>+</sup> is proposed. Thus, the exceedingly reactive CF<sub>3</sub><sup>+</sup> species can be generated much easier than the CH<sub>3</sub><sup>+</sup> species, contrary to the common sense that CF<sub>3</sub><sup>+</sup> is extremely difficult to generate in solution

RX(48) OF 381 ...AQ + CM ==> CN





CN  
YIELD 93%

RX(48) RCT AQ 220351-08-6

STAGE(1)  
SOL 75-09-2 CH2Cl2  
CON 70 minutes, -90 - -100 deg C

STAGE(2)  
RCT CM 62-53-3  
SOL 75-09-2 CH2Cl2  
CON 3 hours, -90 deg C -> -10 deg C

PRO CN 2070-47-5

NTE irradiated at 253.7nm - first stage, photochemical (first stage)  
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 13 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 145:188529 CASREACT Full-text  
TITLE: Rhodium-Catalyzed Ring-Opening Reactions of  
N-Boc-Azabenzonorbornadienes with Amine  
Nucleophiles

AUTHOR(S): Cho, Yong-hwan; Zunic, Valentin; Senboku, Hisanori;  
Olsen, Madeline; Lautens, Mark

CORPORATE SOURCE: Davenport Laboratories, Department of Chemistry,  
University of Toronto, Toronto, ON, M5H 3H6, Can.

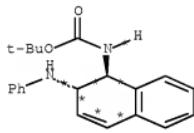
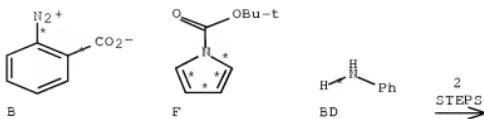
SOURCE: Journal of the American Chemical Society (2006),  
128(21), 6837-6846

PUBLISHER: CODEN: JACSAT; ISSN: 0002-7863  
American Chemical Society

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB In the presence of a rhodium catalyst (5 mol %) generated *in situ* from [Rh(cod)Cl]<sub>2</sub> and (S,S')-(R,R')-C<sub>2</sub>-ferriphos, the asym. ring-opening reaction of azabenzonorbornadienes with various aliphatic and aromatic amines proceeded with high enantioselectivity ( $\leq 99\% \text{ ee}$ ) to give 1,2-dihydronaphthalene-1,2-diamines in high yields. In the specific case of pyrrolidine as nucleophile, Et<sub>3</sub>NHCl was necessary as an additive for good reactivity and enantioselectivity. Addnl., a practical protocol was developed for the ring-opening of N-*tert*-butoxycarbonyl-7-azabenzonorbornadiene with volatile amines at elevated temps. and standard pressure, using R2NH.HI and (Me<sub>2</sub>CH)<sub>2</sub>NET. The exptl. results showed that the nature of the chiral ligand has the significant impact on the reactivity of the catalyst and the use of excess amount (2.2 equiv to Rh) of the chiral ligand plays an important role to improve the enantioselectivity in the present asym. reaction.

RX(57) OF 98 COMPOSED OF RX(2), RX(20)  
RX(57) B + F + BD ==> BE



BE  
YIELD 96%

RX(2) RCT B 1608-42-0, F 5176-27-2  
PRO G 5176-28-3  
SOL 107-06-2 C1CH2CH2Cl  
CON SUBSTAGE(1) 45 minutes, 60 deg C  
SUBSTAGE(2) 60 deg C -> room temperature

RX(20) RCT G 5176-28-3, BD 62-53-3  
PRO BE 897439-87-1  
CAT 12092-47-6 Rh COD Cl dimer, 126108-99-4 Ferrocene,  
1,1'-bis[(1S)-1-(dimethylamino)ethyl]-2,2'-  
bis(diphenylphosphino)-, (2S,2'S)-  
CON 30 hours, 80 deg C  
NTE no solvent, stereoselective

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 144:311953 CASREACT [Full-text](#)  
TITLE: Synthesis of thiazolidin-4-one derivatives on the

basis of  $\alpha$ -substituted thiocyanates  
AUTHOR(S): Ostapiuk, Yuri V.; Matiychuk, Vasyl S.; Obushak, Mykola D.

CORPORATE SOURCE: Department of Organic Chemistry, Ivan Franko National University of Lviv, Lvov, 79005, Ukraine

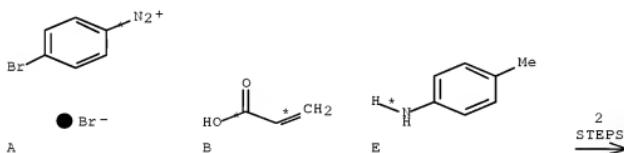
SOURCE: International Electronic Conferences on Synthetic Organic Chemistry, 5th, 6th, Sept. 1-30, 2001 and 2002  
[and] 7th, 8th, Nov. 1-30, 2003 and 2004 (2004),

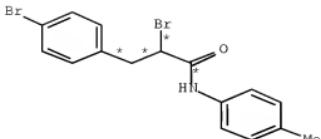
1707-1712. Editor(s): Seijas, Julio A. Molecular  
Diversity Preservation International: Basel, Switz.  
CODEN: 69GTCO  
DOCUMENT TYPE: Conference; (computer optical disk)  
LANGUAGE: English  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A conference. 2-Bromo-3-(4-bromophenyl)propionic acid has been obtained by interaction of 4-bromobenzene diazonium bromide with acrylic acid (catalyst - CuBr). 2-Bromo-3-(4-bromophenyl)propionic acid has been used for the synthesis of amides, e.g. I. 5-(4-Bromobenzyl)-2-imino-3-R1-thiazolidin-4-ones, e.g. II, have been obtained on account of intramol. reaction by the nucleophilic substitution of bromine by thiocyanate ion of these amides. By the reaction of arenediazonium chlorides with acrolein (catalyst - CuCl2) the 3-aryl-2-chloropropanals have been synthesized. By the interaction of 3-aryl-2-chloropropanals with thiourea, 5-R-benzyl-2-aminothiazoles, e.g. III, have been obtained, that have been transformed to corresponding N-(5-R-benzylthiazol-2-yl)-2-chloroacetamides, e.g. IV, by action of chloroacetyl chloride. N-(5-R-benzylthiazol-2-yl)-2-chloroacetamides are ring closing under action of thiocyanate ion and form 3-substituted 2-iminothiazolidin-4-ones, e.g. V. By alkylation of benzothiazole-2-thiol and morpholine with N-(5-R-benzylthiazol-2-yl)-2-chloroacetamides, corresponding N-(5-R-benzylthiazol-2-yl)-2-(benzothiazol-2-yl)thioacetamides, e.g. VI, and 4-(5-R-benzylthiazol-2-yl)-4- morpholinecarboxamide have been obtained.

RX(35) OF 91 COMPOSED OF RX(1), RX(2)  
RX(35) A + B + E ==> F





F  
YIELD 67%

RX(1) RCT A 2008-62-2, B 79-10-7  
 PRO C 857813-94-6  
 CAT 7787-70-4 CuBr  
 NTE Meerwein arylation

RX(2) RCT C 857813-94-6

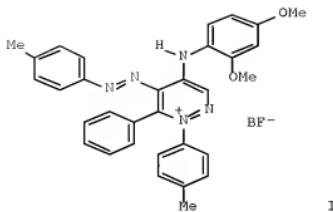
STAGE(1)  
 RGT G 7719-09-7 SOC12

STAGE(2)  
 RCT E 106-49-0

PRO F 879497-64-0

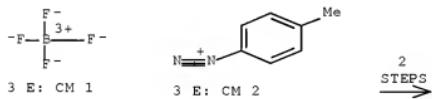
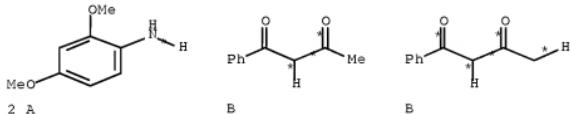
REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

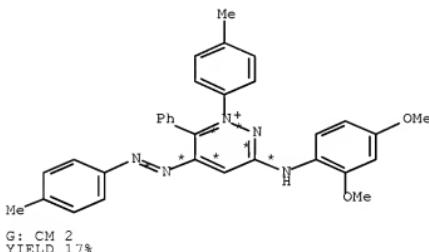
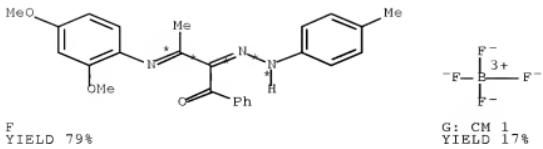
L5 ANSWER 4 OF 13 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 142:219222 CASREACT Full-text  
 TITLE: Formation of pyridazinium salts by azo coupling of  
 N-substituted 3-amino-1-phenylbut-2-en-1-ones and  
 diazonium salts  
 AUTHOR(S): Simunek, Petr; Peskova, Marketa; Bertolasi, Valerio;  
 Lycka, Antonin; Machacek, Vladimir  
 CORPORATE SOURCE: Department of Organic Chemistry, University of  
 Pardubice, Pardubice, 53210, Czech Rep.  
 SOURCE: European Journal of Organic Chemistry (2004), (24),  
 5055-5063  
 CODEN: EJOCFK; ISSN: 1434-193X  
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Treatment of 3-(2,4-dimethoxyphenylamino)- and 3-methylamino-1-phenylbut-2-en-1-ones with some benzenediazonium tetrafluoroborates gave 1,4,5,6-tetrasubstituted pyridazinium tetrafluoroborates, e.g., I. The pyridazinium salts have been identified by X-ray anal. and by their 1H, 13C, 15N, 11B, and 19F NMR spectra. Their formation is most probably the result of nucleophilic attack on the carbonyl carbon by the nitrogen of the hydrazone group and subsequent dehydration.

RX(7) OF 10 COMPOSED OF RX(1), RX(2)  
 RX(7) 2 A + 2 B + 3 E ==> E + G





RX(1) RCT A 2735-04-8, B 93-91-4

PRO C 387832-31-7

SOL 108-88-3 PhMe

CON 3 hours, reflux

RX(2) RCT C 387832-31-7, E 459-44-9

RGT H 127-09-3 AcONa

PRO F 843613-91-2, G 843613-95-6

SOL 75-09-2 CH2Cl2

CON 72 hours, room temperature

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 142:176480 CASREACT Full-text

TITLE: 2-Alkyl-1,2,3,4-benzotetrazinium tetrafluoroborates:

Their reaction with nucleophiles

AUTHOR(S): Lipilin, Dmitry L.; Smirnov, Oleg Y.; Churakov, Aleksandr M.; Strelenko, Yuri A.; Tyurin, Aleksei Y.; Ioffe, Sema L.; Tartakovskiy, Vladimir A.

CORPORATE SOURCE: N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, 119991, Russia

SOURCE: European Journal of Organic Chemistry (2004), (23), 4794-4801

CODEN: EJOCKF; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

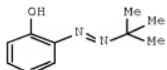
DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI



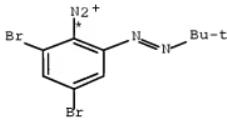
I

AB Treatment of 2-alkyl-1,2,3,4-benzotetrazinium tetrafluoroborates with a variety nucleophiles, at room temperature, resulted in elimination of an N<sub>2</sub> mol. to afford ortho-substituted azobenzenes, e.g., I. This reaction could be suitable for mild phenylation of carboxylic acids and other compds. containing active hydrogen. A plausible reaction pathway for the reaction is discussed.

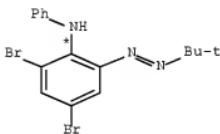
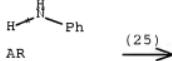
RX(25) OF 39      E + AR ==&gt; AS



E: CM 1



E: CM 2

AS  
YIELD 97%

RX(25)      RCT E 832076-38-9, AR 52-53-3

PRO AS 832077-20-0

SOL 75-09-2 CH<sub>2</sub>C<sub>12</sub>

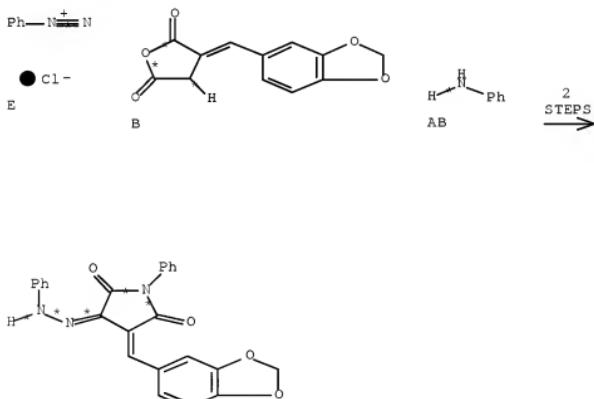
CON 10 minutes, 20 deg C

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS

## RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 13 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 139:214429 CASREACT Full-text  
 TITLE: Synthesis of azo-coupled etaconic acid anhydride and its reactions with nucleophiles  
 AUTHOR(S): Prabhu, P. J.; Bhise, N. B.; Dave, M. A.  
 CORPORATE SOURCE: Department of Chemistry, K.J. Somaiya College of Science and Commerce, Mumbai, 400 077, India  
 SOURCE: Asian Journal of Chemistry (2003), 15(2), 634-638  
 PUBLISHER: Asian Journal of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB 3-Methylenedioxy-benzylidene succinic anhydride was condensed with diazonium salts of various aromatic amines to form hydrazones or dyes which were further treated with nucleophiles like 10% NaOH and NaBH4 to give various pyrazolinone derivs., resp. and cyclic imide derivs. of the corresponding hydrazones. The antibacterial and antifungal activities of some the products are also reported.

RX(24) OF 45 COMPOSED OF RX(2), RX(14)  
 RX(24) E + B + AB ==> AC



AC  
 YIELD 64%

RX(2) RCT E 100-34-5

STAGE(1)

RGD G 7647-01-0 HCl, H 7632-00-0 NaNO<sub>2</sub>  
SOL 7732-18-5 Water  
CON 15 minutes, 0 deg C

STAGE(2)  
RCT B 99971-42-3  
SOL 67-64-1 Me<sub>2</sub>CO  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 30 minutes, 0 deg C

PRO F 587881-56-9

RX(14) RCT F 587881-56-9, AB 62-53-3

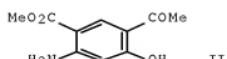
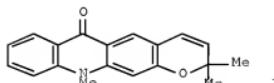
STAGE(1)  
SOL 64-17-5 EtOH  
CON 4 - 5 hours, reflux

STAGE(2)  
CAT 7647-01-0 HCl  
SOL 7732-18-5 Water  
CON room temperature

PRO AC 587881-78-5

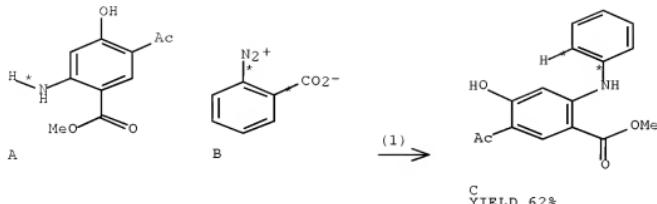
REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 13 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 139:85518 CASREACT Full-text  
TITLE: Regioselective synthesis of demethoxyisoacronycine involving nucleophilic addition to benzyne  
AUTHOR(S): Rudas, Monika; Nyerges, Miklos; Toke, Laszlo; Groundwater, Paul W.  
CORPORATE SOURCE: Research Group of the Hungarian Academy of Sciences, Department of Organic Chemical Technology, Technical University of Budapest, Budapest, H-1521, Hung.  
SOURCE: Heterocycles (2003), 60(4), 817-824  
PUBLISHER: Japan Institute of Heterocyclic Chemistry  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Demethoxyisoacronycine (I) was prepared in seven steps using the nucleophilic addition of aniline derivative II to benzyne as a key step.

RX(1) OF 32      A + B ==> C...

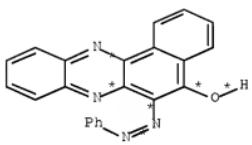
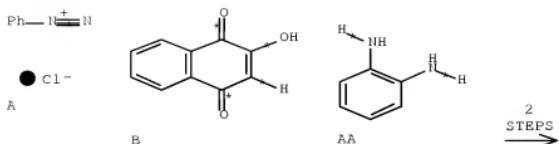


RX(1)      RCT A 71407-97-1, B 1608-42-0  
PRO C 250644-93-0  
SOL 75-09-2 CH2C12  
CON reflux

REFERENCE COUNT:      13      THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5      ANSWER 8 OF 13      CASREACT      COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER:      138:4399      CASREACT [Full-text](#)  
TITLE:      Synthesis and Transformations of  
2-Hydroxy-3-arylazo-1,4-naphthoquinones  
AUTHOR(S):      Romanyuk, A. L.; Polishchuk, O. P.; Litvin, B. L.;  
Ganushchak, N. I.  
CORPORATE SOURCE:      Franko State University, Lvov, Ukraine  
SOURCE:      Russian Journal of General Chemistry (Translation of  
Zhurnal Obschhei Khimii) (2002), 72(2), 251-254  
PUBLISHER:      MAIK Nauka/Interperiodica Publishing  
DOCUMENT TYPE:      Journal  
LANGUAGE:      English  
AB      A series of 2-hydroxy-3-arylazo-1,4-naphthoquinones was prepared by coupling of 2-hydroxy-1,4-naphthoquinone with aryl diazonium chlorides. The reactivity of the products toward electrophilic and nucleophilic agents was studied. In reaction with o-phenylenediamine they give condensation products, the corresponding benzo[a]phenazines.

RX(15) OF 17 COMPOSED OF RX(1), RX(12)  
RX(15)      A + B + AA ==> AB



AB  
YIELD 63%

RX(1) RCT A 100-34-5

STAGE(1)

RGT D 144-55-8 NaHCO<sub>3</sub>  
 SOL 7732-18-5 Water  
 CON 0 - 5 deg C

STAGE(2)

RCT B 83-72-7  
 RGT D 144-55-8 NaHCO<sub>3</sub>  
 SOL 7732-18-5 Water  
 CON - 1.5 hour

STAGE(3)

RGT E 7647-01-0 HCl  
 SOL 7732-18-5 Water

PRO C 476682-15-2

RX(12) RCT AA 95-54-5, C 476682-15-2  
 PRO AB 68839-40-7  
 SOL 64-17-5 EtOH  
 CON 2 hours, reflux

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 9 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

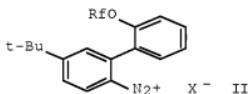
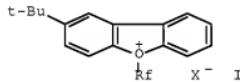
ACCESSION NUMBER: 130:168232 CASREACT Full-text

TITLE: Preparation of O-(perfluoroalkyl)dibenzofuranium salts

as perfluoroalkylating agents and their intermediates  
 such as (perfluoroalkoxy)biphenyldiazonium salts  
 INVENTOR(S): Umemoto, Teruo; Adachi, Kenji; Ishihara, Sumi  
 PATENT ASSIGNEE(S): Daikin Industries Ltd., Japan  
 SOURCE: PCT Int. Appl., 49 pp.  
 CODEN: PIXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906389	A1	19990211	WO 1998-JP3416	19980730
W: JP, US RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1013651	A1	20000628	EP 1998-935301	19980730
EP 1013651	B1	200070530		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
AT 363477	T	20070615	AT 1998-935301	19980730
US 6239289	B1	20010529	US 2000-463706	20000215
PRIORITY APPLN. INFO.:			JP 1997-207901	19970801
			WO 1998-JP3416	19980730

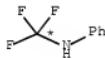
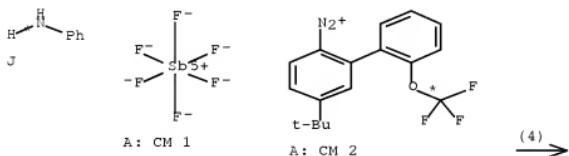
OTHER SOURCE(S): MARPAT 130:168232  
 GI



AB O-(Perfluoroalkyl)dibenzofuranium salt derivs. represented by general formula (I; Rf is perfluoroalkyl being 1 to 10 carbon atoms; and X- is a conjugate based of a Bronsted acid) are prepared by cyclization of (perfluoroalkoxy)biphenyldiazonium salts (II; Rf and X- are defined as above) and are used as perfluoroalkylating agents for perfluoroalkylation of nucleophiles containing O or N, e.g. amines and alcs. When the O-(perfluoroalkyl)dibenzofuranium salt derivs. are used as perfluoroalkylating agents, they permit high-yield perfluoroalkylation, and are applicable to a wide range of compds. and inhibited in self-decomposition as to be relatively stable. The presence of tert-Bu at 5-position improves the stability of I and thereby usefulness of I as perfluoroalkylating agents. Thus, a solution of 7.17 g 2-amino-5-tert-butyl-2'-(trifluoromethoxy)biphenyl in 46 mL Et2O was cooled to -78° with stirring, followed by adding 6.47 g nitrosonium hexafluoroantimonate (ON+SbF6-), and the resulting mixture was warmed to 10° over 3 h in an warm bath, while adding 10 mL Et2O when temperature reached to

5°, to give 58% II (Rf = CF<sub>3</sub>, X<sup>-</sup> = SbF<sub>6</sub><sup>-</sup>) (III). A CCl<sub>2</sub>D<sub>2</sub> solution of 6.5 mg III in a Pyrex NMR tube was cooled to -106° and irradiated by a high pressure Hg lamp (400 W and 253.7 nm) for 45 min to give I (Rf = CF<sub>3</sub>, X<sup>-</sup> = SbF<sub>6</sub><sup>-</sup>) (IV) 87, 5-tert-butyl-2-fluoro-2'-(trifluoromethoxy)biphenyl 8, and 5-tert-butyl-2-chloro-2'-(trifluoromethoxy)biphenyl 3% according to <sup>19</sup>F- and <sup>1</sup>H-NMR anal. at -80°. When the temperature was gradually raised to -30°, IV completely decomposed to CF<sub>4</sub> and 2-tert-butylbenzofuran. To the cold (-99° to -90°) reaction mixture similarly prepared were added variety of alcs. and amines. When phenecyl alc. was added at -90°, the resulting mixture was warmed to -10° over 3 h to give 80% phenecyl trifluoromethyl ether. Although in general, diazonium salts are explosive in nature, III has .apprx.27° higher decomposition temperature (84.7-85.8°) compared to that of the 4-tert-Bu regioisomer (m.p. 58-60°) and can be handled at room temperature, and safely stored and transported.

RX(4) OF 9      J    +    A    ==>    K



K  
YIELD 81%

RX(4)      RCT J 62-53-3, A 220351-08-6

PRO K 2070-47-5

SOL 75-09-2 CH2Cl2

NTE two-step reacti

REFERENCE COUNT:      1      THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5    ANSWER 10 OF 13    CASREACT    COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:      110:192508    CASREACT Full-text

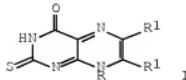
TITLE:      Pteridines. Part LXXXVII. Synthesis and properties of 8-substituted 2-thiolumazines

AUTHOR(S):      Huebsch, Walter; Pfleiderer, Wolfgang  
CORPORATE SOURCE:      Fak. Chem., Univ. Konstanz, Konstanz, D-7750, Fed. Rep. Ger.

SOURCE:      Helvetica Chimica Acta (1988), 71(6), 1379-91

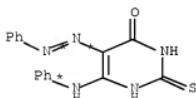
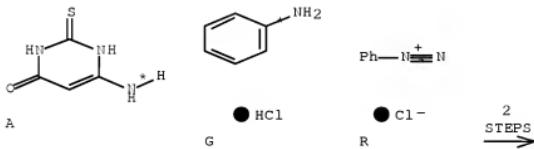
DOCUMENT TYPE:  
LANGUAGE:  
GI

CODEN: HCACAV; ISSN: 0018-019X  
Journal  
English



AB 2,8-Dihydro-2-thioxopteridin-(3H)-ones I (R = Me, CH<sub>2</sub>CH<sub>2</sub>OH, Ph; R1 = H, Me, Ph) and their S-Me derivs. have been synthesized by condensation of 5-amino-6-(substituted amino)-1,2-dihydro-2-thioxopyrimidin-4(3H)-ones and the S-Me derivs. with RICOCORI. The presence of a quinonoid cross-conjugated  $\pi$ -electron system makes this type of compound susceptible to nucleophilic addns. in position 7, which leads to intramol. and intermol. covalent adducts.

RX(43) OF 124 COMPOSED OF RX(3), RX(10)  
RX(43) A + G + P ==> W



W  
YIELD 89%

RX(3) RCT A 1004-40-6, G 142-04-1  
PRO H 98421-02-4

RX(10) RCT H 98421-02-4, R 100-34-5  
 RGT N 1310-73-2 NaOH  
 PRO W 120270-10-2  
 SOL 7732-18-5 Water, 64-17-5 EtOH

L5 ANSWER 11 OF 13 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 100:155992 CASREACT [Full-text](#)  
 TITLE: Reactions of (aryloxy)oxosulfonium ylides with carbonyl compounds  
 AUTHOR(S): Okuma, Kentaro; Nakanishi, Kazuto; Ohta, Hiroshi  
 CORPORATE SOURCE: Dep. Chem., Fukuoka Univ., Fukuoka, 814-01, Japan  
 SOURCE: Journal of Organic Chemistry (1984), 49(8), 1402-7  
 CODEN: JOCEAH; ISSN: 0022-3263  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB (Aryloxy)oxosulfonium salts and alkylolithiums give ylides which add to carbonyl compds. to give  $\beta$ -(aryloxy) sulfones (I)  $\beta$ -(aryloxy) sulfones (II), and  $\alpha,\beta$ -unsatd. or  $\beta,\gamma$ -unsatd. sulfones in 1.4-17.9, 1.2-7.2, and 4.5-13.5% yields, resp. The ylides reacted with the carbonyl compds. to give betaines which formed unusual 4-membered cyclic alkoxyoxyosulfonium salts containing aryloxy anions. The aryloxy anions thus formed attacked the  $\beta$ -C of these salts to give I; the aryloxy anions, which might be formed by autoxidn., also attack the  $\beta$ -C of these salts to give II. Deprotonation at C( $\alpha$ ) or C( $\gamma$ ) by these anions gave the unsatd. sulfones. This is the first example in which an ylide reacts with carbonyl compds. to give sulfones via a 4-membered cyclic alkoxyoxyosulfonium salt which was formed in an intramol. SN2 reaction. To yields of unsatd. sulfones were raised to 35-60% in a one-pot reaction.

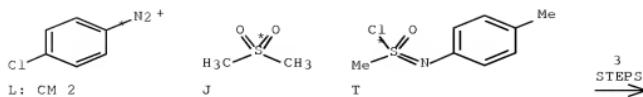
RX(48) OF 48 COMPOSED OF REACTION SEQUENCE RX(12), RX(21), RX(13)  
 AND REACTION SEQUENCE RX(9), RX(1), RX(13)

... P + Q ==> T...  
 ... L + J + T ==> U



L: CM 1

START NEXT REACTION SEQUENCE



U  
YIELD 77%

RX(12) RCT P 106-49-0, Q 676-85-7  
PRO R 19977-37-8  
CAT 121-44-8 Et3N

RX(21) RCT R 19977-37-8  
RGT AF 7782-50-5 C12  
PRO T 89278-81-9

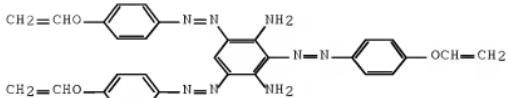
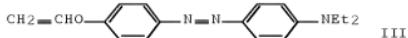
RX(9) RCT L 673-41-6, J 67-71-0  
PRO A 73040-88-7

RX(1) RCT A 73040-88-7  
PRO B 106-48-9  
CAT 104-87-0 4-MeC6H4CHO

RX(13) RCT T 89278-81-9, B 106-48-9  
PRO U 89278-82-0

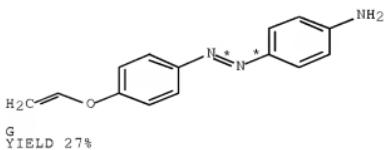
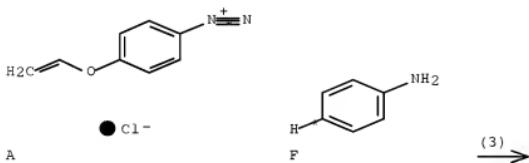
L5 ANSWER 12 OF 13 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 97:162482 CASREACT Full-text  
 TITLE: (Vinylxyloxy)benzenediazonium chloride in reactions of  
 nitrogen coupling and the exchange of the diazo group  
 with nucleophilic reagents  
 AUTHOR(S): Stepanova, Z. V.; Grebneva, P. I.; Skvortsova, G. G.  
 CORPORATE SOURCE: Inst. Org. Khim., Irkutsk, USSR  
 SOURCE: Zhurnal Organicheskoi Khimii (1982), 18(8), 1711-15  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian  
 GI



AB 4-CH<sub>2</sub>:CHOC<sub>6</sub>H<sub>4</sub>N<sub>2</sub><sup>+</sup>Cl<sup>-</sup> (I) underwent azo coupling with PhNH<sub>2</sub>, PhNMe<sub>2</sub>, PhNEt<sub>2</sub>, and 1,3-C<sub>6</sub>H<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub> (II) to give, e.g., III; with II di- and tri-coupling products (e.g., IV) were also obtained. Reactions with HgCl<sub>2</sub> and CuCl were also studied; with CuCN I and its m-isomer gave the corresponding nitriles.

RX(3) OF 9 A + F ==> G



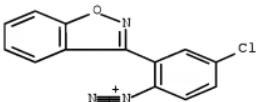
RX(3) RCT A 34649-14-4, F 62-53-3  
PRO G 83300-43-0

ACCESSION NUMBER: 83:164108 CASREACT [Full-text](#)  
TITLE: Nucleophilic displacement of aromatic  
fluorine. I. Synthesis of benzisoxazoles  
AUTHOR(S): Walser, Armin; Flynn, Thomas; Fryer, R. Ian  
CORPORATE SOURCE: Chem. Res. Dep., Hoffmann-La Roche Inc., Nutley, NJ,  
USA  
SOURCE: Journal of Heterocyclic Chemistry (1974), 11(6), 885-8  
CODEN: JHTCAD; ISSN: 0022-152X  
DOCUMENT TYPE: Journal  
LANGUAGE: English

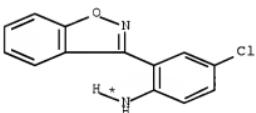
GI For diagram(s), see printed CA Issue.

AB The quinazoline 3-oxides I (R = H, Cl) convert to the  
benzisoxazoloquinazolines II by heating in Ac<sub>2</sub>O. The dihydroquinazoline-3-  
oxides III underwent aromatization under the same conditions. Hydrolysis of I  
or II gave the 3-(2-aminophenyl)benzisoxazoles IV which could be rearranged to  
the 3-(2-hydroxyphenyl)indazoles V with hydride. Possible mechanisms are  
discussed.

RX(12) OF 39 ...T + N ==> U

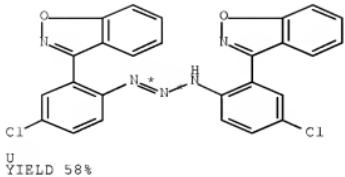


T: CM 2



(12) →

H



YIELD 58%

RX(12) RCT T 340203-43-2, N 55076-00-1  
PRO U 55076-03-4

=> log off  
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF  
LOGOFF? (Y)/N/HOLD:y  
STN INTERNATIONAL LOGOFF AT 10:10:24 ON 20 OCT 2008